

ANALYSIS OF THE TRAJECTORY OF A SPHERE MOVING THROUGH A GEOMETRIC CONSTRICTION

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ABSTRACT. We present a numerical study of the effect of inertia on suspended particles moving through a geometric constriction to understand the behavior of particles in analogous microfluidic settings, such as pinched flow fractionation devices. The particles are driven by a constant force in a quiescent fluid, and the constriction (the *pinching gap*) corresponds to the space between a plane wall and a second, fixed sphere of the same size (the *obstacle*). The results show that, due to the effect of inertia and geometric constriction (individual or combined) the particles attain smaller surface-to-surface separations from the obstacle. We then relate the minimum surface-to-surface separation to the effect that the short-range repulsive non-hydrodynamic interactions (such as solid-solid contact due to surface roughness, electrostatic double layer repulsion, etc.) would have on the particle trajectories. In particular, using a simple hard-core repulsive potential model for such interactions, we infer that the particles would experience larger lateral displacements moving through the pinching gap, as inertia increases and/or the aperture created by the constriction decreases. Thus, separation of particles based on the differences in density is in principle possible, owing to differences in inertia associated with them. However, we observe in the simultaneous presence of pinching wall and significant inertia, that the wall reduces inertia effects and hinders separation.

1. INTRODUCTION

The deterministic motion of spherical particles through geometric constrictions is at the core of a number of microfluidic unit operations and devices. Some prominent examples include separation systems, e.g., based on pinched flow fractionation,[1] particle focusing

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methods,[2] such as geometrical focusing,[3] and constricted microchannels and micromodels of porous media used to study particle deposition and clogging.[4, 5] In all cases, the interactions of the suspended particles with the confining walls of a microfluidic channel play a crucial role in determining their motion and fate. The nature of the interactions can be hydrodynamic, particularly important when particle size is comparable to the confinement, or non-hydrodynamic, such as solid-solid contact due to surface roughness.

The motion of suspended particles in microfluidic systems is in many cases described based on the fluid flow streamlines obtained in the absence of particles. Rigorously, such an explanation is valid only for point particles, because it neglects the effect of particle size and particle-wall hydrodynamic interactions. Moreover, the streamlines are calculated in the Stokes regime, neglecting fluid inertia. Particle inertia is also ignored and the effect of non-hydrodynamic interactions, such as solid-solid contact, is typically incorporated indirectly. For example, Jain and Posner model the effect of roughness on particle dispersion in order to estimate the relevant statistical properties of the separation process, such as its resolution.[6] However, there is ample evidence that hydrodynamic interactions, inertia effects, and non-hydrodynamic repulsive forces significantly affect the individual particle trajectories through narrow constrictions, leading to the separation process.[7, 9, 8]

Consider the case of pinched flow fractionation (PFF), in which the separative lateral displacement experienced by particles of unequal size is achieved by passing the suspension through a constriction, followed by a sudden expansion.[1, 10, 11, 6, 12, 13] Although the original explanation offered for the separative lateral displacement was based on particle motion superimposed on the streamlines in Stokes flow,[1] particle size and hydrodynamic interactions cannot be ignored in PFF due to the small particle-wall separations that take place near the constriction.[7, 8] It has been also shown recently, that inertia effects (manifesting themselves as ‘lift’ forces) might play a crucial role in PFF.[8] In some particle focusing methods inertial effects are also present, and even exploited as a suspension of particles moves through a series of constrictions.[14, 2] In fact, the asymmetric trajectories observed in focusing devices in which the constriction is fore-aft symmetric[3] indicates the presence of *irreversible* forces, i.e., inertial forces or non-hydrodynamic interactions between the particles and the channel wall. Otherwise, the trajectories should be symmetric and reversible, consistent with Stokes equations. In the case

of clogging in microchannels, it has been argued that particle deposition involves the interplay between hydrodynamic as well as non-hydrodynamic interactions.[4] The hydrodynamic interaction of particles with constrictions/channel walls leads to particle trajectories that deviate from flow streamlines, and if a particle reaches a critical separation from the wall, non-hydrodynamic attractive interactions result in particle deposition.[4, 5]

In this work, we investigate the motion of a spherical particle passing through a constriction created by a spherical obstacle of the same size and a plane wall (see figure 1). We are interested in the minimum surface-to-surface separation occurring between the particle and the obstacle during the motion, since it is the relevant length scale to assess the relative importance of short-range non-hydrodynamic interactions between them. Specifically, we show that the minimum separation decreases as the magnitude of inertia increases and/or the aperture created by the constriction decreases. The inferences drawn from these results are consistent with the observations reported in previous experiments, in that, the lateral displacement of a given size of particles increases as the aperture of the constriction becomes smaller.[15] In addition, the computational nature of the work presented here enables us to isolate the effects of fluid and particle inertia by adjusting both the particle-to-fluid density ratio as well as the force acting on the particle. In comparison, the ratio of the densities was moderate in the experiments reported in Ref. [15] ($O(10^0) - O(10^1)$), and hence the effects of particle and fluid inertia were coupled.

The article is organized as follows: in the following section, we define the geometry of the system under investigation and describe the parameter space relevant to the problem in terms of dimensionless numbers. In §3, we introduce a hard-core model for non-hydrodynamic repulsive interactions, and discuss its effect on particle trajectories in the absence (3.1) and presence (3.2) of inertia. In §4, we present the results of our simulations in the presence of a pinching wall only (4.1), in the presence of inertia only (4.2), and both in the presence of a pinching wall as well as significant inertia (4.2.1). Finally in §5 we summarize the inferences drawn from this work.

2. SYSTEM DEFINITION AND PARAMETER SPACE

A schematic view of the system under consideration is shown in figure 1. A spherical particle suspended in a quiescent fluid moves past a spherical obstacle of the same radius a (diameter d) under the action of a constant force. The x -axis is set in the direction of the constant

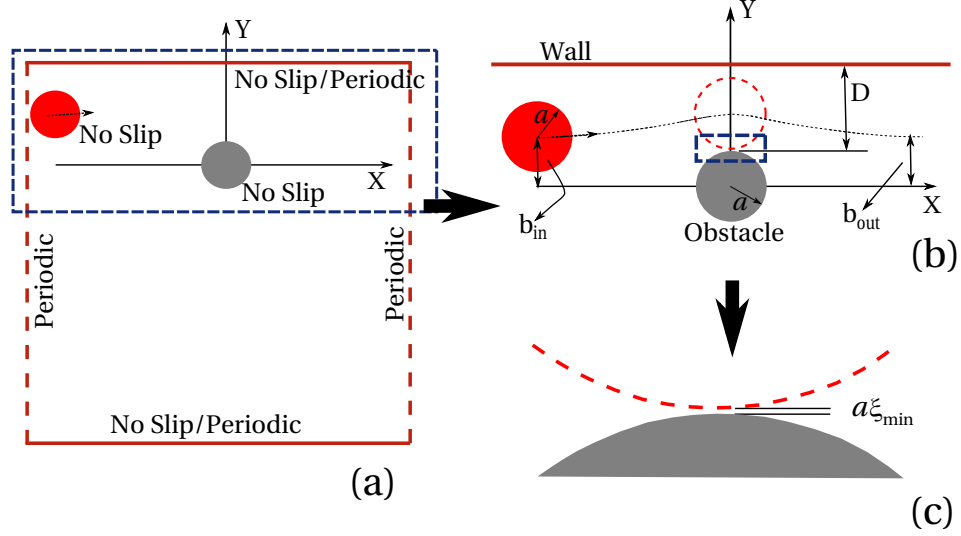


FIGURE 1. (a) System, simulation box and boundary conditions. The schematic is to scale, i.e., the box is 16 obstacle/particle radii in length. The top wall creates the pinching gap. In the absence of walls, we use the periodic boundaries for the box, and the obstacle is at the center of the box. (b) The part of the simulation box indicated with dashed lines in (a) is enlarged here. The initial offset b_{in} , the final offset b_{out} and the aperture of the pinching gap D are indicated. The dashed circle depicts the position of the particle when the particle-obstacle separation is minimum (in the absence of inertia). (c) Enlarged view of the particle (dashed) and the obstacle (solid) surfaces showing the minimum separation $a\xi_{min}$ between them.

force, and the far upstream (downstream) – i.e., $x \rightarrow -\infty$ ($x \rightarrow +\infty$) – position of the particle along the y -axis is the *initial offset* b_{in} (*final offset* b_{out}). A plane wall perpendicular to the positive y -axis creates a wall-obstacle *pinching gap* of minimum aperture D . The motion of a particle initially located in the xy -plane is confined to that plane, due to the symmetry of the problem. The minimum value of the dimensionless surface-to-surface separation between the particle and the obstacle for a given trajectory is ξ_{min} (the corresponding dimensional separation is $a\xi_{min}$ as shown in figure 1(c)).

Numerical simulations are performed using the lattice Boltzmann method (*susp3d*).[16, 17, 18] The boundary conditions imposed in the

simulations are shown in figure 1(a): no-slip at all fluid-solid interfaces, periodic boundary conditions in x and z directions, as well as in y -direction in the absence of the pinching wall. The size of the simulation box is $16a$ in all directions (particle radius $a = 5$ lattice units). We vary the aperture of the pinching gap D by translating the obstacle center along the y direction. The initial position of the particle, upstream to the obstacle ($x_0 \approx -7a$), is given by the initial offset b_{in} , and the final offset is calculated at the symmetric position with respect to the y -axis. Here we note that the code implementing the lattice Boltzmann method is designed to construct a channel, such that two walls are simultaneously added on the opposite faces of the simulation box (for example, see the top and bottom walls in figure 1(a)). However, preliminary simulation tests showed that in a sufficiently large box (i.e., $16a$ in x, y and z directions in this work), the effect of the wall opposite to the pinching wall is negligible.

The parameter space for our investigation is characterized by three dimensionless numbers: the Reynolds number Re , quantifying fluid inertia, the Stokes number St , quantifying particle inertia, and the ratio of the particle diameter to the aperture of the pinching gap d/D , quantifying the extent of pinching. We define the Reynolds and Stokes numbers based on the bulk (Stokes) settling velocity and the radius of the particle,

$$(1) \quad Re = \frac{aU_{Stokes}}{\nu} = \frac{a}{\nu} \left(\frac{2}{9} \cdot \frac{\rho_p}{\rho_f} \cdot \frac{a^2 g}{\nu} \right),$$

$$(2) \quad St = \frac{\tau_p}{\tau_f} = \frac{2}{9} \cdot \frac{\rho_p}{\rho_f} Re = ag \left(\frac{2}{9} \cdot \frac{\rho_p}{\rho_f} \cdot \frac{a}{\nu} \right)^2,$$

where $\tau_p = m/6\pi\mu a$ is the inertial relaxation time for an isolated suspended particle,[19] $\tau_f = a/U_{Stokes}$ is the characteristic time of the flow around the particle, ν is the kinematic viscosity of the fluid ($\nu = 1/6$ in lattice units throughout this work¹), g is the acceleration due to

¹It has been reported that using kinematic viscosity $\nu = 1/6$ (in lattice units) hastens the simulations as well as reduces numerical errors [Ladd, A. J. C. and Verberg, R. (2001), J Stat Phys, Vol.104, Nos. 5/6, pp. 1191–1251], providing a basis for our choice. Also, we note that the accuracy of the lattice-Boltzmann method based on the inherent compressibility, is reported to be $O(Ma^2)$ in the literature [e.g., Ladd, A. J. C. and Verberg, R. (2001), J Stat Phys, Vol.104, Nos. 5/6, pp. 1191-1251 and Hazi, G. (2003), Phys Rev E, Vol. 67, article 056705], where Ma is the Mach number associated with the system. For our system, the largest instantaneous particle velocities observed in the simulations are $O(10^{-2}$ lattice units). Given that the LB-code is D3Q19, velocity of sound is given by $c_s^2 = 1/3$ in lattice units. Thus,

the constant external force acting on the particle,² and ρ_p , ρ_f are the densities of the particle and the fluid, respectively. We cover a range of Re and St values from negligible ($O(10^{-4})$ - $O(10^{-3})$) to appreciable ($O(0.1)$ - $O(1)$) by varying ρ_p/ρ_f and g , and use four values of the d/D ratio: 0.588, 0.5, 0.4 and 0.333.

In general, the trajectories followed by the particles for different initial offsets b_{in} , and thus the minimum dimensionless separations ξ_{min} , are functions of the three dimensionless numbers: Re , St , d/D . We estimate the effect of short-range non-hydrodynamic interactions on a particle trajectory by comparing the range of the interactions with the corresponding minimum separation attained by the particle along that trajectory. Further, the particle trajectories in the Stokes regime are symmetric about the y -axis in the absence of non-hydrodynamic interactions. Therefore, the symmetry (or equivalently, asymmetry) exhibited by a particle trajectory also serves a diagnostic purpose: any asymmetry present in the trajectories obtained in our simulations is indicative of deviations from the Stokes regime (i.e., significant inertia)[9, 22]. The presence of such asymmetry can be determined by comparing the initial and final offsets. Thus, in the next sections, we use the minimum separation (ξ_{min}) as well as the offsets (b_{in} and b_{out}) as representative variables to investigate the effect of non-hydrodynamic interactions, in the presence of inertia and pinching on the particle trajectories. Throughout this article, for brevity and clarity, we present results corresponding to $b_{in} = 2a$. In the supplementary information, we present our results for the entire range of b_{in} considered ($1.6a$ - $2.2a$), and showing the minimum separation (ξ_{min}) as a function of the offsets b_{in} and b_{out} for all cases in terms of the aperture of the pinching gap and inertia.

3. HARD-CORE MODEL FOR NON-HYDRODYNAMIC INTERACTIONS

3.1. Stokes regime and the critical offset. We have shown in previous work that the minimum separation ξ_{min} decreases dramatically with the initial offset b_{in} , especially when b_{in} becomes comparable to the obstacle radius (or, the mean of particle and obstacle radii for unequal particle and obstacle sizes).[22, 24] An initial offset of $b_{in} \sim a$,

$Ma \sim O(10^{-2})$ and errors related to inherent compressibility of the method are $O(10^{-4})$.

²We note that, in our simulations we specify the constant external acceleration acting on the particle, which is multiplied by the particle mass to compute the net force acting on it. Therefore, the expression for the Stokes settling velocity in equation 1 contains just the particle density ρ_p , and not the difference between the particle and fluid densities, $\Delta\rho = \rho_p - \rho_f$.

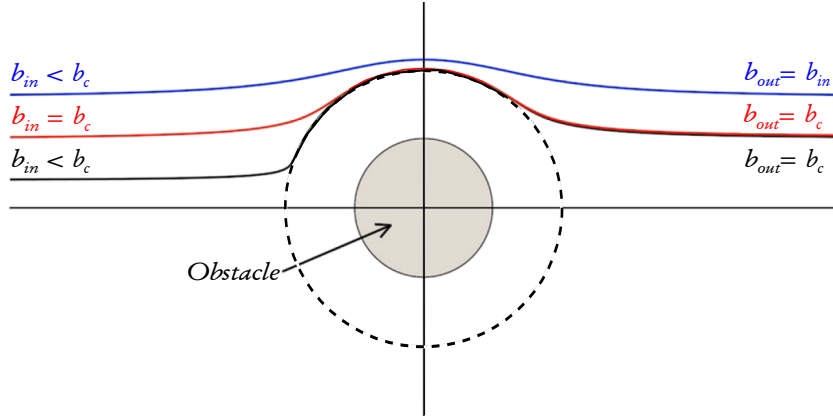


FIGURE 2. Trajectories corresponding to the three possible types of particle-obstacle ‘collisions’, adapted from Ref [9]. The particle travels from left (incoming half of the trajectory) to right (outgoing half of the trajectory). The dashed circle represents the excluded volume inaccessible to the particle centers.

for example, results in a minimum separation $\xi_{min} \sim O(10^{-3})$. Therefore, for a particle with its radius in the millimeter range, the corresponding minimum separation amounts to a few microns, while for micrometer-sized particles, the predicted minimum separations are at atomic length-scales. In reality, micrometer-sized particles exhibit various repulsive non-hydrodynamic interactions at separations $O(100 \text{ nm})$, such as, electrostatic double layer repulsion,[25] solid-solid contact due to surface roughness[26, 27] and steric repulsion.[28] Following previous studies, we use a simple model that describes these interactions with a hard-core repulsive potential.[22, 29, 30, 31, 32] In this approximation, if the dimensionless range of the repulsive interaction is ϵ , any surface-to-surface separation $\xi < \epsilon$ is not possible, since it is inside the core of the interaction. Consequently, if a particle trajectory attains a minimum separation ξ_{min} in the absence of non-hydrodynamic interactions, by comparing it with ϵ we investigate the effect of these interactions. Moreover, we assume that the hard-core repulsion is the only effect of the potential, in that, the hydrodynamic mobility of the suspended particle is not affected by the interaction.[22, 29, 30, 31, 32]

In the absence of inertia, there is a one-to-one relationship between the minimum separation and the initial offset. [22, 24] We can thus define a *critical* offset b_c , as the final offset resulting from a minimum separation equal to the range of the repulsive interaction i.e., $\xi_{min} = \epsilon$ (see

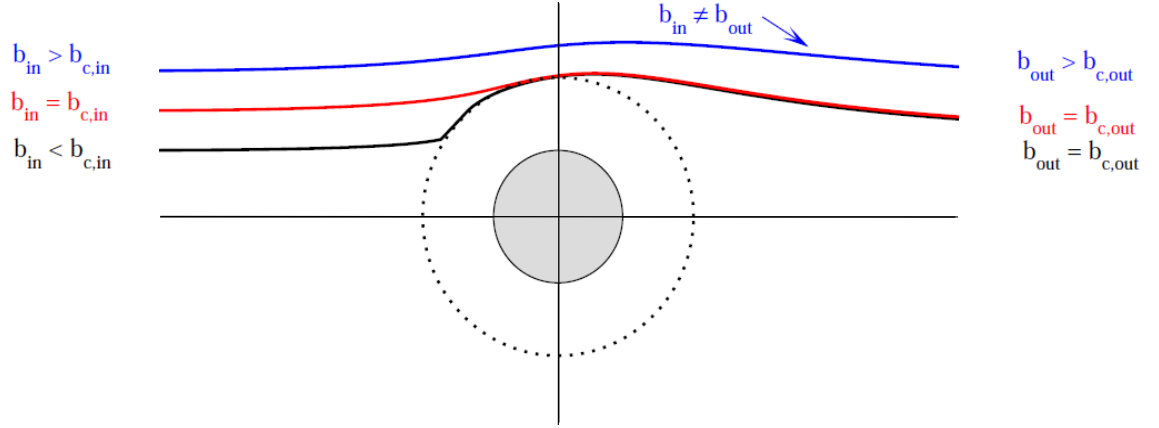


FIGURE 3. In presence of significant inertia (in this particular case, particle inertia, $St = 1.11$), the trajectories are asymmetric even in the absence of non-hydrodynamic interactions. Such asymmetry leads to two critical offsets, viz.- $b_{c,in}$, $b_{c,out}$ as shown.

figure 2). In previous work, we have established that the critical offset b_c completely characterizes the asymmetry caused by the repulsive interaction in the particle trajectory[22, 9]: any trajectory beginning with an initial offset smaller than the critical value ($b_{in} < b_c$) would result in a minimum separation smaller than the range of the repulsive interaction. Since such separations are unattainable in the presence of the interaction, once the particle attains ϵ , the separation remains constant and equal to ϵ on the approaching side and, as shown in figure 2, the outgoing half of the trajectory collapses onto the trajectory with $b_{out} = b_c$. On the other hand, for $b_{in} \geq b_c$, the trajectories, unaffected by non-hydrodynamic interactions, are symmetric in the absence of inertia. The single-valued function relating ξ_{min} and b_{in} (or b_{out}) is the same as that relating ϵ and b_c . [22, 24] Therefore, we can predict the dependence of b_c on the pinching gap for a given ϵ by computing ξ_{min} as a function of b_{in} for different d/D ratios. *In conclusion, the critical offset is a macroscopic and experimentally measurable variable, which serves as a probe/proxy for the range of the repulsive interaction, a microscopic effective variable that is experimentally less accessible.*[24]

3.2. Inertia effects on the critical offset. The fore-aft symmetry of the trajectories is broken in the presence of inertia (see figure 3). Therefore, in the presence of non-hydrodynamic interactions, we need to define two distinct critical offsets: the critical initial-offset $b_{c,in}$ and the critical final-offset $b_{c,out}$, as shown in figure 3. The critical initial-

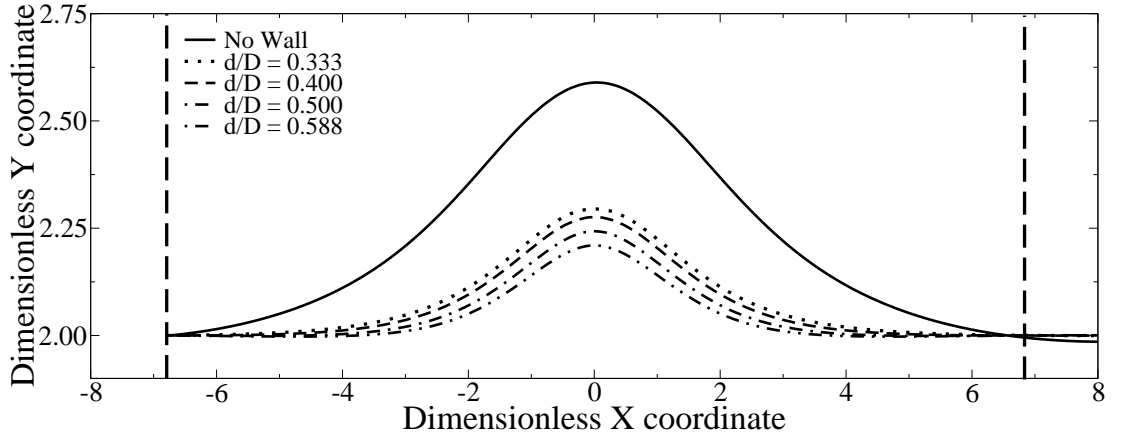


FIGURE 4. Various trajectories with $b_{in} = 2.0$, exhibiting the effect of pinching in the Stokes regime ($Re = 5 \times 10^{-4}$ and $St = 1.11 \times 10^{-4}$). The axes are nondimensionalised by the radius of the particle. The vertical dashed lines at $x \approx \pm 7$ represent the initial and final x -coordinates of the particle, respectively.

offset $b_{c,in}$ is defined in the same manner as in case of negligible inertia. The definition of the critical final-offset ($b_{c,out}$) needs the auxiliary assumption that inertia is negligible when the particle approaches small surface-to-surface separations from the obstacle. Under this assumption, the final offset would also present a critical behavior such that, all trajectories with $b_{in} < b_{c,in}$ would collapse onto a single trajectory downstream to the obstacle, which in turn defines the critical final-offset $b_{c,out}$ corresponding to $b_{c,in}$.

4. RESULTS AND IMPLICATIONS OF THE HARD-CORE MODEL

4.1. Effect of pinching in the Stokes regime. In figure 4, we show representative trajectories corresponding to different apertures of the pinching gap, for the same initial offset $b_{in} = 2a$ and with negligible fluid and particle inertia. As expected, the trajectories remain fore-aft symmetric in all cases. When the aperture of the pinching gap is reduced, we observe that the particle follows trajectories that get significantly closer to the obstacle.

In light of the hard-core model discussed before, let us now consider the effect of the non-hydrodynamic interactions on the trajectories through a pinching gap in the Stokes regime. Consider trajectories with the initial offset $b_{in} = 2a$ (see figure 4), and non-hydrodynamic interactions with a dimensionless range $\epsilon = \epsilon_0$. Let the critical offset

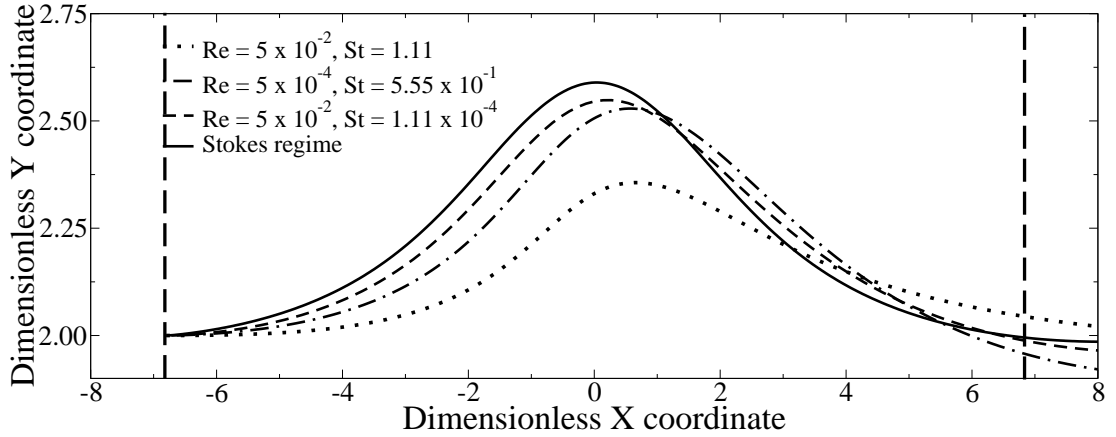


FIGURE 5. Various trajectories with $b_{in} = 2a$, exhibiting the effect of inertia in the absence of pinching. The axes are nondimensionalised by the radius of the particle. The vertical dashed lines at $x \approx \pm 7a$ represent the initial and final x -coordinates of the particle, respectively.

corresponding to ϵ_0 in the absence of pinching be $b_c = b_{c0} < 2a$. Using the arguments in the previous section, in the absence of pinching the particle trajectories under consideration are fore-aft symmetric, attain a minimum separation $\xi_{min} > \epsilon_0$, and the non-hydrodynamic interactions have no effect on them (e.g., the top-most trajectory in figure 2). As the aperture of the pinching gap is reduced, while keeping the initial offset constant at $2a$, figure 4 shows that the particle comes closer to the obstacle. Eventually, at a particular aperture, we get $\xi_{min} = \epsilon_0$, which implies that the critical offset has increased from b_{c0} to $2a$. In other words, *the critical offset that leads to a given minimum separation increases as the aperture of the pinching gap decreases*. This result is in qualitative agreement with our experiments.[15] In the supplementary information,[23] we arrive at the same inference directly by considering the minimum separation ξ_{min} as a function of the initial offset b_{in} (see figures S1 and S2, and the corresponding discussion in the supplementary information[23]).

4.2. Effect of inertia in the absence of pinching. Figure 5 shows representative trajectories (with $b_{in} = 2a$) in the presence of inertia effects, but in the absence of a pinching wall. We observe that the effect of inertia is similar to that of pinching discussed earlier, such that the particle gets closer to the obstacle as the magnitude of (fluid and/or particle) inertia increases. Although the effects of pinching and

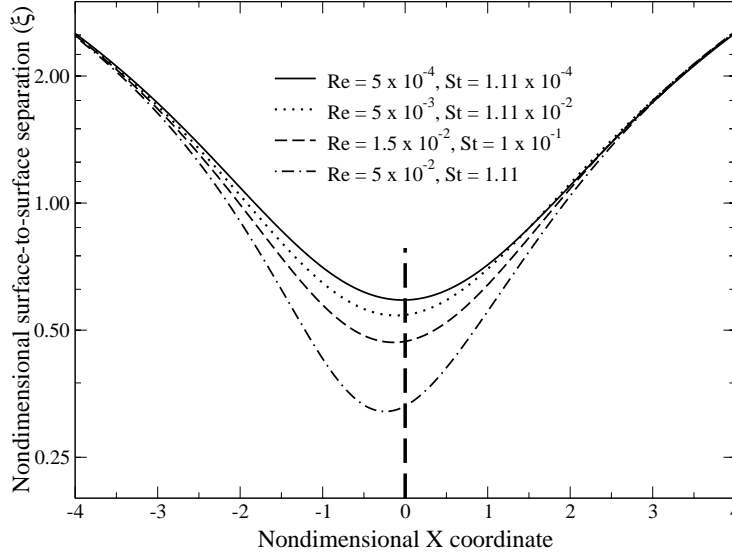


FIGURE 6. The dimensionless surface-to-surface separation between the particle and the obstacle, as a function of the dimensionless x -coordinate of the particle. The plot shows the combined effect of particle and fluid inertia on the dimensionless separation along particle trajectories for $b_{in} = 2a$, in the absence of pinching. The vertical dashed line depicts the symmetry plane of the system at $x = 0$.

inertia on the minimum separation are similar, in the presence of inertia the minimum separation is no longer attained at the symmetry plane ($x = 0$) but upstream to the obstacle-center (at negative x values, see figure 6). We also observe that the x -coordinate at which the minimum separation is attained decreases with increasing inertia (similar plots showing the individual effects of fluid and particle inertia can be found in the supplementary information[23]).

4.2.1. Effect of pinching and inertia. In figure 7, we consolidate our results and present the minimum separation ξ_{min} for all the cases of pinching and inertia considered in this work, at $b_{in} = 2a$. As discussed so far, we observe that reducing the aperture of the pinching gap causes the particle to attain a smaller minimum surface-to-surface separation in all the cases shown, with or without particle and/or fluid inertia. Further, the figure also shows that for any fixed aperture of the pinching gap the minimum separation attained by the particle decreases with increasing inertia. Our simulations also indicate that the effect

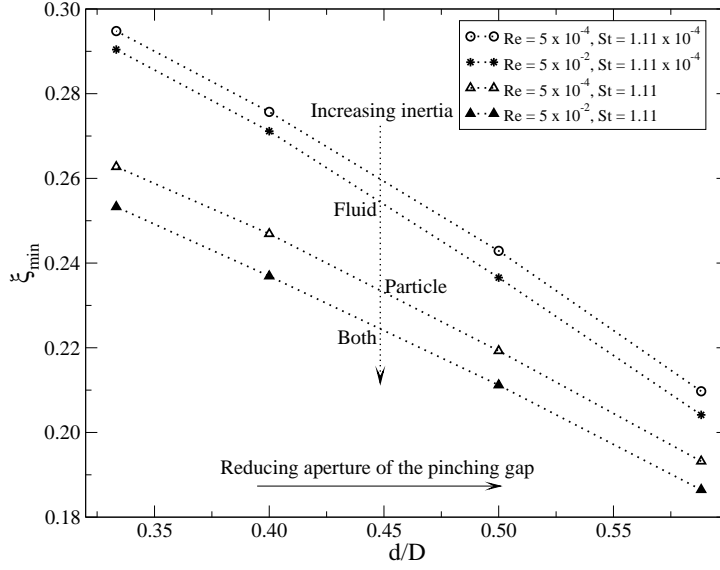


FIGURE 7. Effect of increasing the extent of pinching ($d/D \uparrow$) on the minimum surface-to-surface separation between the particle and the obstacle, for different magnitudes of inertia and a fixed initial offset, $b_{in} = 2a$.

of particle inertia on ξ_{min} is attenuated in the presence of the pinching wall. The attenuation could be due to the hydrodynamic resistance offered by the pinching wall, which reduces the particle velocity, thereby diminishing the effective magnitude of particle inertia (note that for calculating the Stokes numbers reported in this work, we have used the bulk settling velocity of spheres). The detailed plots of ξ_{min} as a function of b_{in} for different Stokes and Reynolds numbers are presented in figures S2 and S3 in the supplementary information.[23] The effect of pinching on these plots is shown in figures S5–S7 in the supplementary information.[23]

We are also interested in the effect of inertia in combination with pinching on the final offset b_{out} , since changes in the final offset as a function of inertia could lead to separation based, for example, on density differences. In figure 8, we present the effects of particle and fluid inertia on the final offset, for $b_{in} = 2a$. In terms of particle inertia, we observe that the final offset decreases with increasing Stokes number. The final offset decreases less when the trajectories undergo pinching, than in the absence of pinching. As mentioned earlier, we suspect that this behavior is to the diminished particle inertia due to the hydrodynamic resistance offered by the wall. In the case of fluid

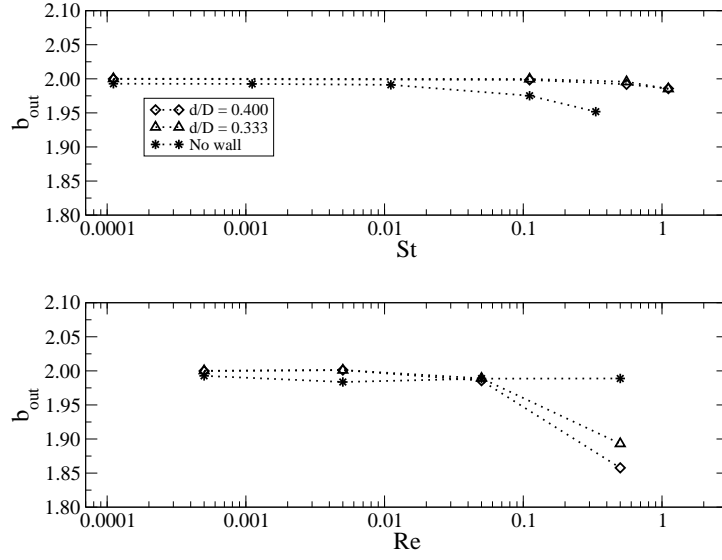


FIGURE 8. The final offset b_{out} (corresponding to $b_{in} = 2a$) as a function of Stokes (top) and Reynolds (bottom) numbers, for different apertures of the pinching gap.

inertia, we observe that for $Re < 0.1$ the final offset is unaffected, irrespective of the presence or absence of the pinching wall. For higher magnitudes of fluid inertia ($Re \sim O(1)$), we observe that the final offset decreases with the aperture of the pinching gap. Such decrease is comparable to the effect of lift forces in the proximity of the pinching wall, which render the final offset ill-defined. In the supplementary information[23] (figures S5, S6 and the accompanying discussion) we present the minimum separation ξ_{min} as a function of the initial offset b_{in} , which is consistent with the attenuation of particle inertia and the presence of lift forces.

Figure 7 shows that the minimum separation decreases for smaller apertures of the pinching gap for a constant magnitude of inertia. Therefore, similar to the discussion in §4.1, we can infer that the critical initial-offset $b_{c,in}$ increases with pinching. Further, the minimum separation also decreases with an increasing magnitude of inertia, for a fixed aperture of the pinching gap. Thus, the critical initial-offset increases with increasing particle inertia (see figures S2 and S5–S7 in the supplementary information[23]). Since $b_{c,out}$ is a monotonically increasing function of $b_{c,in}$, one might expect that $b_{c,out}$ also increases with pinching and inertia. However, figure 8 shows that for a constant b_{in} , the final offset decreases due to the effect of inertia. Due to such

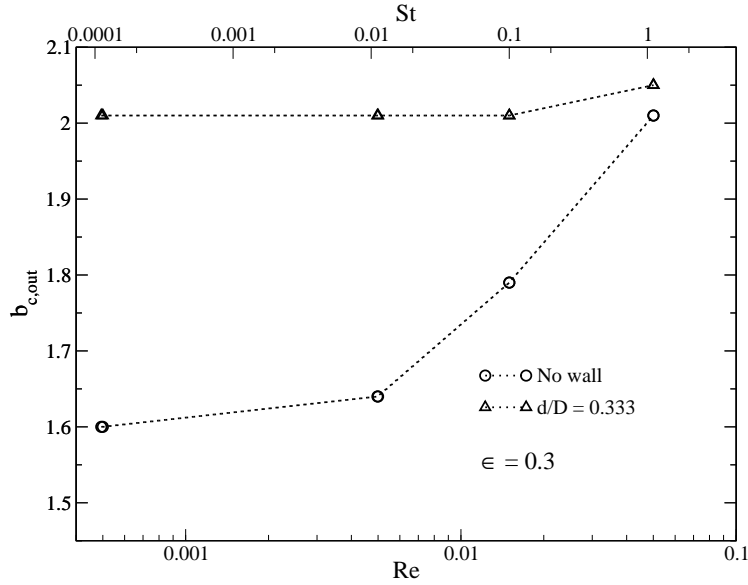


FIGURE 9. The critical final-offset $b_{c,out}$ corresponding to $\epsilon = 0.3$, as a function of Reynolds and Stokes numbers, in the presence and the absence of a pinching wall.

competing effects, commenting on the behavior of the final critical offset as a function of the aperture of the pinching gap and inertia is not trivial. Our simulations indicate, as shown in figure 9, that the critical final-offset $b_{c,out}$ indeed increases with inertia, but the change becomes substantially smaller in the presence of pinching, provided that the effect of lift forces generated due to the pinching wall are minimal (also see ξ_{min} as a function of b_{out} in figures S11 and S12 in the supplementary information[23]).

Thus, in conclusion, *both critical offsets increase with inertia and/or pinching, for a constant range of the non-hydrodynamic interactions $\xi_{min} = \epsilon$* . Thus, in a mixture of particles of the same size, a particle with sufficiently higher density would exhibit larger critical final-offset $b_{c,out}$ than a particle with lower density, thereby rendering its separation possible (assuming that both particles exhibit similar range of non-hydrodynamic interactions). In the presence of a pinching wall, a similar inference can be drawn. Although, the change in the critical offsets due to inertia can be expected to be small because of the attenuation of inertia effects by the wall.

5. SUMMARY

We have shown that in the presence of inertia effects and/or a pinching wall, suspended particles driven around an obstacle by a constant force, get closer to the obstacle due to pinching as well as inertia. The minimum surface-to-surface separation ξ_{min} as a function of the relative pinching d/D quantifies this phenomenon. Augmented with a simple hard-core repulsion model for non-hydrodynamic interactions (such as solid-solid contact due to surface roughness) our observations lead to the definitions of critical initial- and final-offsets. Both offsets are equal when inertia is negligible. The offsets increase upon decreasing the aperture of the pinching gap, and/or upon increasing inertia. When the inertia and pinching effects are combined together, the final offset varies only weakly with inertia. In this case, we surmise that the presence of a pinching wall attenuates the effect of particle inertia. In conclusion, particles with different densities could be separated in systems with significant inertia, more effectively in the absence of pinching than in its presence.

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- [20] Note1. It has been reported that using kinematic viscosity $\nu = 1/6$ (in lattice units) hastens the simulations as well as reduces numerical errors [Ladd, A. J. C. and Verberg, R. (2001), J Stat Phys, Vol.104, Nos. 5/6, pp. 1191–1251], providing a basis for our choice. Also, we note that the accuracy of the lattice-Boltzmann method based on the inherent compressibility, is reported to be $O(Ma^2)$ in the literature [e.g., Ladd, A. J. C. and Verberg, R. (2001), J Stat Phys, Vol.104, Nos. 5/6, pp. 1191–1251 and Hazi, G. (2003), Phys Rev E, Vol. 67, article 056705], where Ma is the Mach number associated with the system. For our system, the largest instantaneous particle velocities observed in the simulations are $O(10^{-2})$ lattice units. Given that the LB-code is D3Q19, velocity of sound is given by $c_s^2 = 1/3$ in lattice units. Thus, $Ma \sim O(10^{-2})$ and errors related to inherent compressibility of the method are $O(10^{-4})$.
- [21] Note2. We note that, in our simulations we specify the constant external acceleration acting on the particle, which is multiplied by the particle mass to compute the net force acting on it. Therefore, the expression for the Stokes settling velocity in equation 1 contains just the particle density ρ_p , and not the difference between the particle and fluid densities, $\Delta\rho = \rho_p - \rho_f$.
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APPENDIX A. SUPPLEMENTARY MATERIAL

A.1. Pinching gap, inertia and minimum separation. Here, we present the results of our simulations in a different manner than the main text by considering the minimum separation ξ_{min} as a function of the initial or final offsets. We present the results with hierarchically increasing the number of variables in the system. First, we show the effect of decreasing the aperture of the pinching gap for negligible fluid and particle inertia (the Stokes regime, figure S1). Then we show the effect of inertia, in the absence of a pinching wall (figures S2 and S3). Finally we present the cases when fluid and/or particle inertia is significant, in the presence of a pinching wall (figures S5, S6 and S7). As discussed in the main text, the relationship between ξ_{min} and b_{in} shown here, is the same as that between the range of the repulsive non-hydrodynamic interactions and the critical offset.[22, 24] Therefore, representing the data in terms of $\xi_{min}-b_{in}$ plots provides additional clarity to the discussion concerning increasing critical offset in the main text.

In figure S1, we present the effect of decreasing the aperture of the pinching gap on the minimum separation ξ_{min} , in the Stokes regime. As noted in the main text, for a given initial offset we observe that ξ_{min} decreases in the presence of a pinching wall. This is seen by comparing the results shown in solid circles with those in open symbols, which correspond to the absence and presence of a pinching wall, respectively. Moreover, comparing the different curves with open symbols, which correspond to different apertures of the pinching gap, it is clear

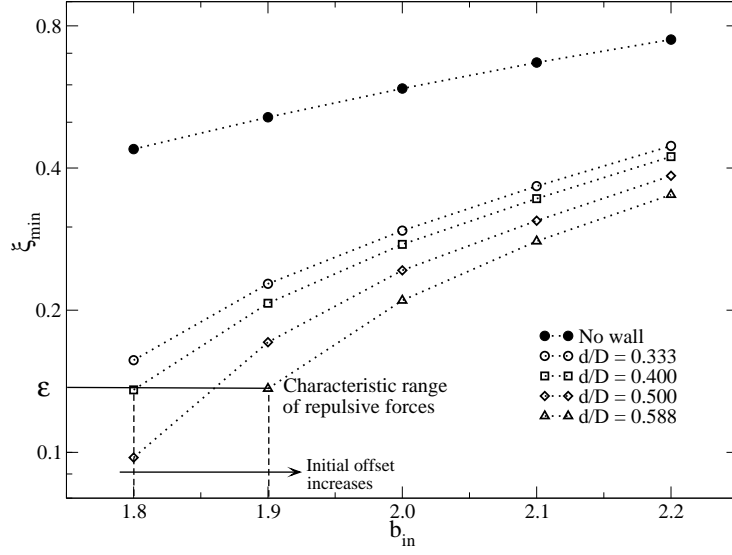


FIGURE S1. The minimum separation ξ_{min} as a function of the initial offset b_{in} , Re and St are negligible.

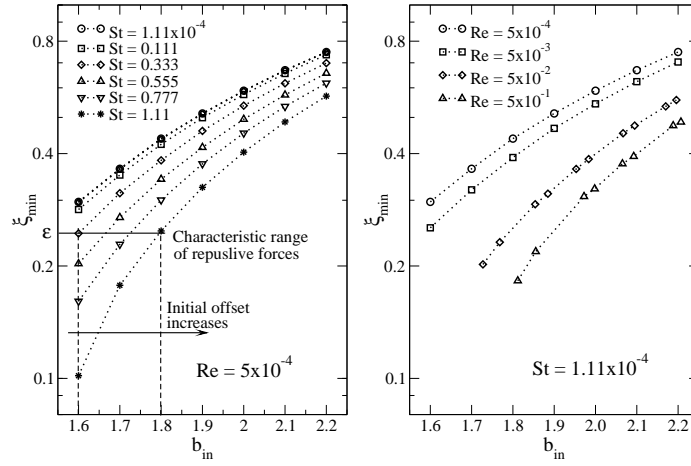


FIGURE S2. The minimum separation ξ_{min} as a function of the initial offset b_{in} , in the absence of pinching. (Left) effect of particle inertia when fluid inertia is negligible, (right) effect of fluid inertia when particle inertia is negligible.

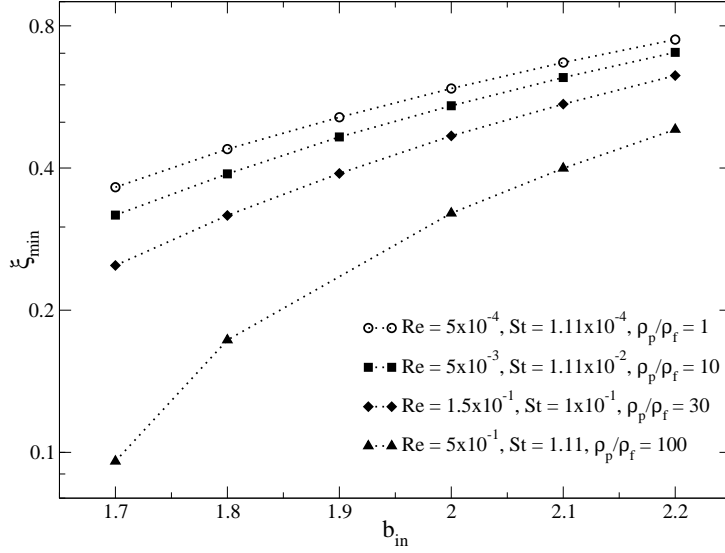


FIGURE S3. The minimum separation ξ_{min} as a function of the initial offset b_{in} showing the effect of significant fluid as well as particle inertia in the absence of pinching.

that decreasing the aperture leads to smaller minimum separations, as the curves shift downwards. Next, in figure S2 we present the effect of inertia in the absence of pinching. The two plots in figure S2 show the effects of fluid and particle inertia on the minimum separation ξ_{min} , independently. It is clear that ξ_{min} decreases when the magnitude of the particle or fluid inertia, increases. The combined effects of particle and fluid inertia are presented in figure S3, where we report results corresponding to particle to fluid density ratios 1, 10, 30, and 100. As explained in the text, inertia causes the particle trajectories to be asymmetric. This leads to the minimum separation taking place before $x = 0$. This is corroborated in figure S4 for fluid and particle inertia acting independently. It also shows that the x -coordinate at which the minimum separation is attained, decreases with increasing inertia.

In figures S5 and S6, we present the combined effect of increasing Re or St for apertures of the pinching gap given by $D = 3d$ ($d/D = 0.333$) and $D = 1.7d$ ($d/D = 0.588$), respectively. The plot on the left in each figure shows the effect of increasing St for a fixed aperture of the pinching gap and Re . The plot on the right in each figure shows the effect of increasing Re for the same aperture of the pinching gap and

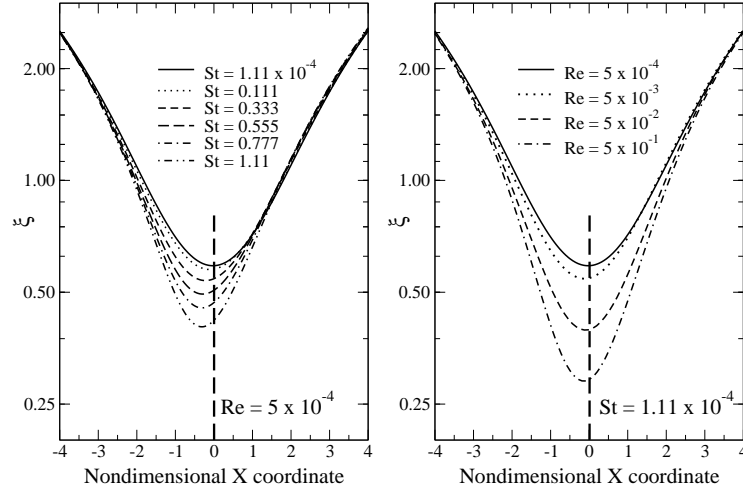


FIGURE S4. The dimensionless surface-to-surface separation ξ as a function of the dimensionless x -coordinate of the particle. The x -coordinate at which the minimum separation is attained along a trajectory, varies with inertia. (Left) Effect of particle inertia, (right) effect of fluid inertia. The minimum separation is attained before the $x = 0$ symmetry-plane in both cases.

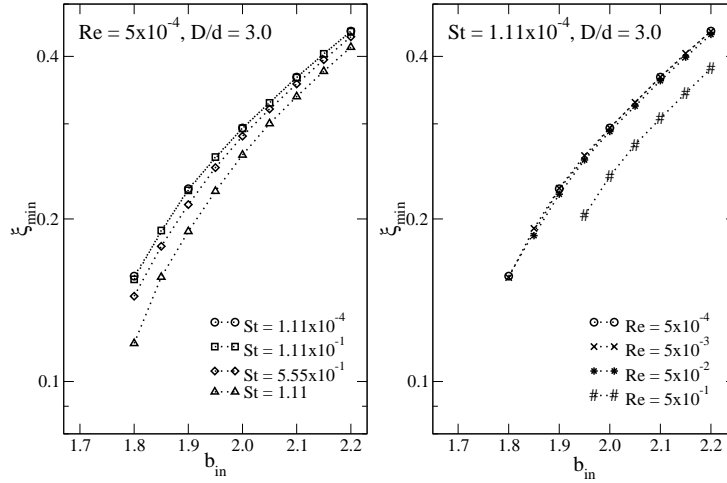


FIGURE S5. The effect of inertia in the presence of a pinching wall, on the $\xi_{min}-b_{in}$ relationship. The aperture of the pinching gap is $3d$ (i.e., $d/D = 0.333$). (Left) The effect of particle inertia, (right) the effect of fluid inertia.

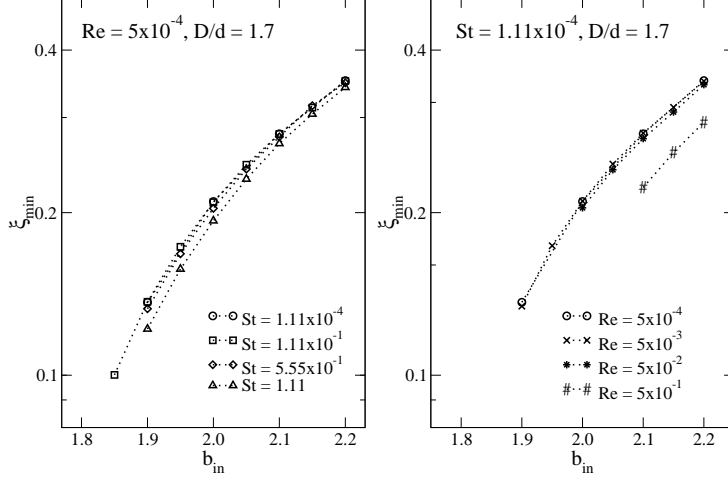


FIGURE S6. The effect of inertia on the $\xi_{min}-b_{in}$ relationship, in the presence of pinching. The aperture of the pinching gap is $1.7d$ (i.e., $d/D = 0.588$). (Left) The effect of particle inertia, (right) the effect of fluid inertia.

constant St . For $b_{in} = 2a$, the corresponding data is presented in figure 7 of the main text. We observe in both cases, that the minimum separation decreases with increasing inertia. In the case of a constant Re (i.e., increasing St), we see that decreasing aperture of the pinching gap (comparing figures S5 and S6) attenuates the effect of inertia on the minimum separation for a fixed initial offset. The decrease in minimum separation (between two magnitudes of inertia) for a given initial offset is smaller when the aperture of the pinching gap is decreased. In contrast, the effect of increasing Re seems to increase as the aperture of the pinching gap becomes smaller, specifically for $Re \sim O(1)$. In this case, however, we observe significant *lift* due to particle-wall interaction, which makes the discussion in terms of offsets less relevant. Note that for $Re \neq 0$ there are no asymptotic offsets, and we observe that for $Re \sim O(1)$ the effect of lift becomes significant over the length of the system.

Finally, representative examples of the combined effect of varying all Re , St and d/D are shown in figure S7. The plot on the left shows the results corresponding to four pairs of St and Re for $d/D = 0.333$. These pairs correspond to the density ratios mentioned earlier, $\rho_p/\rho_f = 1, 10, 30, 100$, for a constant force acting on the particle. The plot on the right presents the minimum separation for the same pairs of Re

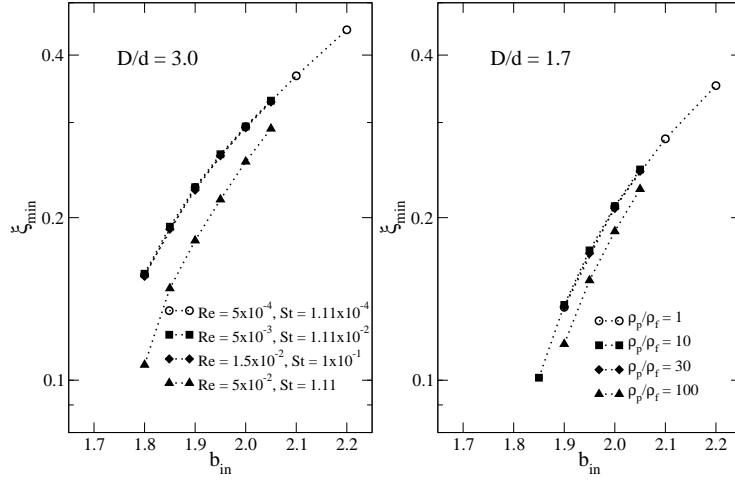


FIGURE S7. Combined effect of the pinching wall, particle and fluid inertia on the ξ_{min} - b_{in} relationship. (Left) the aperture of the pinching gap is $3d$ (i.e., $d/D = 0.333$), (right) the aperture is $1.7d$ (i.e., $d/D = 0.588$).

and St but for, $d/D = 0.588$. The results follow that, increasing inertia effects (both particle and fluid inertia) leads to smaller minimum separations for a fixed initial offset. Also analogous to the results discussed earlier, increasing the extent of pinching decreases the minimum separation corresponding to a given initial offset, but attenuates the relative reduction in minimum separation due to inertia effects.

A.2. Minimum separation, critical offsets and non-hydrodynamic interactions. Similar to the discussion in the main text, here we present the effect that inertia and a pinching wall have on the critical final-offset of the particle trajectories. It is clear from the results discussed both in the main text as well as in the previous section that the minimum separation ξ_{min} decreases when the aperture of the pinching gap is reduced, or the magnitude of inertia is increased, or both. Using the ξ_{min} - b_{in} plots introduced in the previous section, we elaborate more on the idea of the critical initial-offset $b_{c,in}$, and the effect of pinching and/or inertia on it. Further, extending the method, we plot ξ_{min} as a function of the final offset b_{out} for various cases of pinching and inertia, and comment on the behavior of the critical final-offset $b_{c,out}$.

Consider figure S1 in light of the hard-core model of the non-hydrodynamic repulsive interactions explained in the main text. For a fixed range of

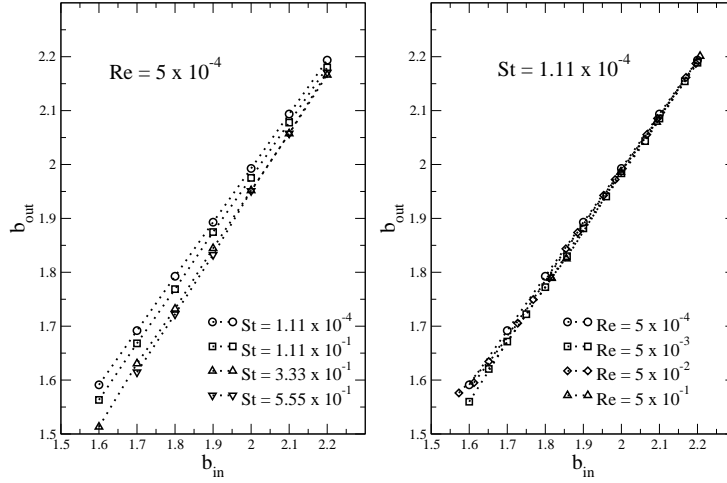


FIGURE S8. The outgoing offset b_{out} as a function of the incoming offset b_{in} . (Left) effect particle inertia, (right) effect of fluid inertia.

the interactions ϵ , we have explained in the main text that the critical final-offset completely characterizes the lateral displacement of the particle downstream of the obstacle. Given that the case presented in figure S1 corresponds to negligible inertia (Stokes regime), both critical initial- and final-offsets are equal. Thus, figure S1 can also be interpreted as a plot of ϵ versus b_c , and clearly shows that the critical offset b_c increases with decreasing aperture of the pinching gap. Similar conclusions can be drawn concerning the critical initial-offset in absence of a pinching wall using figures S2 and S3, that is, the critical initial-offset increases for a fixed range of the repulsive interactions, with increasing magnitude of inertia (fluid and/or particle inertia).

The asymmetry imparted to the particle trajectories by particle inertia, is readily seen in figure S8. This figure supplements the information provided in figures 3 and 5 in the main text. We observe that, in the absence of a pinching wall, the final offset decreases with increasing particle inertia, while fluid inertia has a weak influence on it. As a result, the effect of inertia competes with the effect of pinching and inertia (decreasing the final offset for a given initial offset), as discussed in the main text (in the context of the dependence of $b_{c,out}$ on pinching and inertia). Figures S9 and S10 present the effect of inertia on the minimum separation, as a function of the final offset, and complement figures S2 and S3 respectively. These figures show that the critical final-offset increases with the magnitude of inertia for a constant range

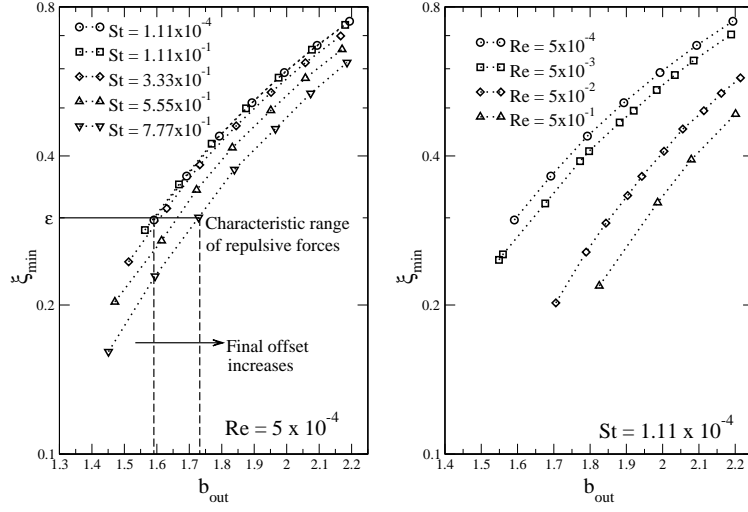


FIGURE S9. The minimum separation as a function of the final offset, (left) effect of particle inertia, (right) effect of fluid inertia.

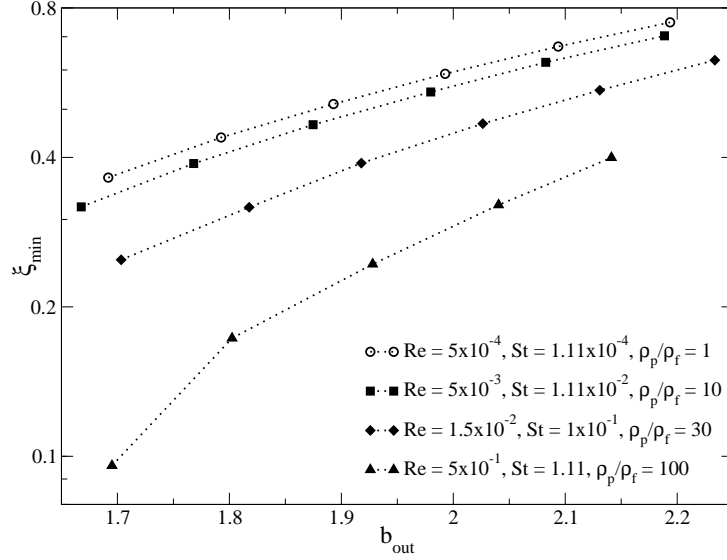


FIGURE S10. Effect of both significant fluid as well as particle inertia on the ξ_{min} - b_{out} relationship, in the absence of pinching.

of the repulsive interactions, ϵ . The presence of both pinching as well as inertia poses the most complex case for analysis, especially, when non-hydrodynamic repulsive forces also play a role. Figures S11 and

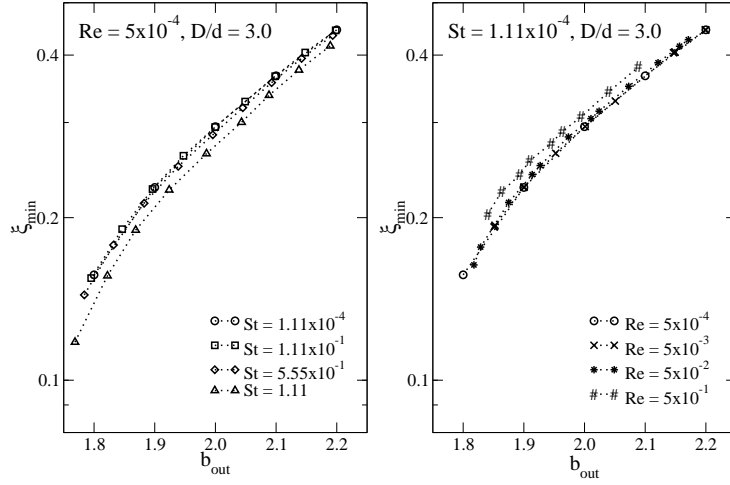


FIGURE S11. The individual effect of particle and fluid inertia in the presence of pinching, on the $\xi_{min}-b_{out}$ relationship. The aperture of the pinching gap is $3.0d$ (i.e., $d/D = 0.333$). (Left) The effect of particle inertia, (right) the effect of fluid inertia.

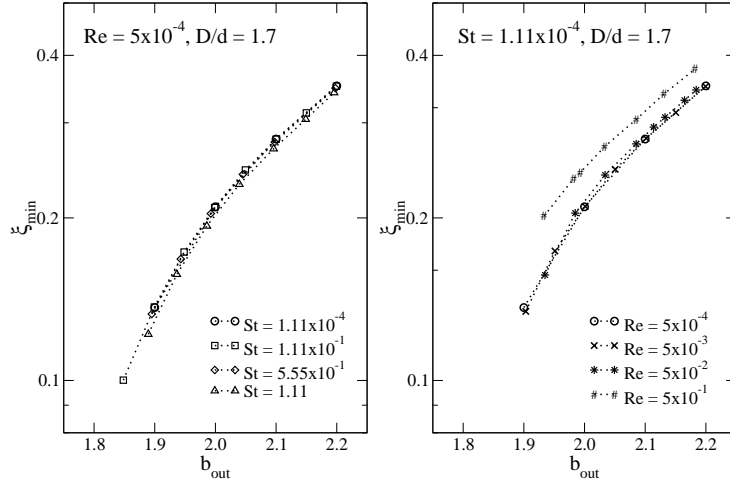


FIGURE S12. The individual effect of particle and fluid inertia in the presence of pinching, on the $\xi_{min}-b_{out}$ relationship. The aperture of the pinching gap is $1.7d$ (i.e., $d/D = 0.588$). (Left) The effect of particle inertia, (right) the effect of fluid inertia.

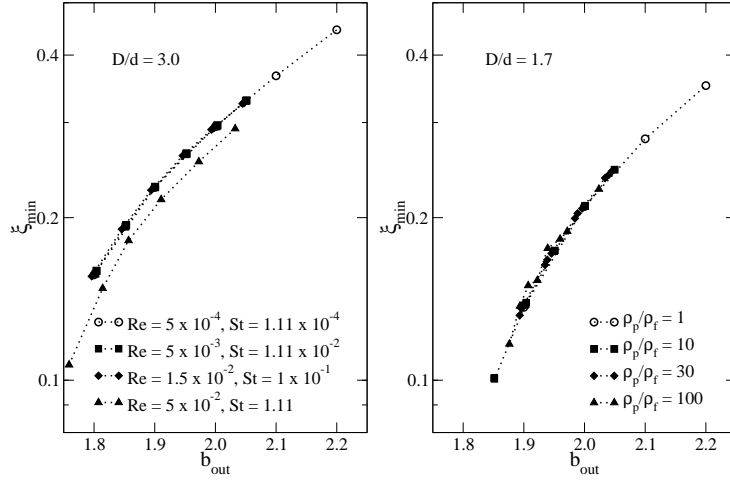


FIGURE S13. The effect of inertia on the $\xi_{min}-b_{out}$ relationship, in the presence of pinching for two different apertures of the pinching gap. (Left) The aperture of the pinching gap is $3.0d$ (i.e., $d/D = 0.333$), (right) the aperture is $1.7d$ (i.e., $d/D = 0.588$).

S12 are analogous to figures S5 and S6. Again, we see that the effect of pinching is to reduce the minimum separation and that the effect of inertia is small, except for $Re \sim O(1)$, where we observe a reversal of the usual trend, with high inertia leading to smaller values of the final offset. As discussed in the main text, this is caused by lift forces, that reduce the final offset, and is therefore a case that should be considered separately.